Table of Timings

Table 1. Timings, in minutes, for direct single-processor MP2 calculations. The molecule is an intermediate (PO_3^-)-$OHCH_3$ [+ $4H_2O$]. There are 14 core, 49 occupied orbitals, and 118 basis functions. The basis set is 6-31G. Memory requirement is minimal.

Job/Machine	Cray (SV1)	HP-UX	PC cluster(Tux)	Origin 3800	IBMP690
Nproc=1	20.9 3.8	2.1	2.3	1.4	

Table 2. Timings, in minutes, for direct single-processor and four-processor distributed MP2 calculations. The molecule is an intermediate (PO_3^-)-$OHCH_3$ [+ $4H_2O$]. There are 14 core, 49 occupied orbitals, and 254 basis functions. The basis set is 6-31G(d,p)+. The serial jobs were run using 800 Mbytes (300 Mbytes on the HP-UX). The four-processor jobs were run with 640 Mbytes per processor.

Job/Machine	Cray (SV1)	HP-UX	PC cluster(Tux)	Origin 3800	IBMP690
Nproc=1	347.0	86.5[c]	38.9	40.2 20.7	
Nproc=4	78.9 -	12.9[a]/	12.5[b]	10.9	5.5

[a] Run over 2 nodes with 2 CPUs per node.

[b] Run over 4 nodes with 1 CPU per node.

[c] Longer time partly because other serial jobs were run with 800 Mwords and only 300 Mwords was available on this machine.

Table3. Timings, in minutes, for non-Direct single-processor and Direct four-processor MCSCF calculations. The molecule is CF_4^{+}. There are 16 core orbitals, 9 active orbitals, 9 active electrons. Number of Basis functions = 75. The MCSCF converges in about 30 steps. Serial job requires not more than 20 Mbytes. Direct four-processor requires 400 Mbytes per CPU as integrals are not read from disk at each step.

Job/Machine	Cray (SV1)	HP-UX	PC cluster(Tux)	Origin 3800	IBMP690
Non-Direct, nproc=1	68.7	12.1	9.9	8.6	4.3
Direct, nproc=4	55.2	-	7.2[a]/7.0[b]	7.5	4.2

[a] Run over 2 nodes with 2 CPUs per node.

[b] Run over 4 nodes with 1 CPU per node.

Table 4. Timings, in minutes, for non-Direct single-processor and Direct four-processor MCSCF calculations. The molecule is ^{6}A Mn(salen)$^-$. There are 53 core orbitals, 11 active orbitals, and 13 active electrons. Number of basis functions = 273. Only two MCSCF steps are timed. The non-direct serial calculation requires 2.0 Gbytes, the direct method uses a total of 1.3 Gbytes per CPU.

Job/Machine	Cray (SV1)	HP-UX	PC cluster(Tux)	Origin 3800	IBMP690
Non-Direct, nproc=1	a	b	b	221.9	107.4

Direct, nproc=4	a	b	b	47.4	48.1

[a] Would take too long.

[b] Not enough memory on each node.

Table 5. Timings, in minutes, for serial SOCI calculations. The system is H_20, the reference is a FORSII wavefunction (1 core, 8 active, 8 active electrons) in which all singles and doubles excitations are allowed, including from the core. There are 74 944 772 determinants. The job requires 6 Gbytes.

Job/Machine	**Cray (SV1)**	**HP-UX**	**PC cluster(Tux)**	**Origin 3800**	**IBMP690**
Nproc=1	-	-	-	500	132